

State-dependent Jastrow correlation functions for ^4He nuclei

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Abstract

We calculate the ground-state energy for the nucleus ^4He with V4 nucleon interactions, making use of a Jastrow description of the corresponding wavefunction with *state-dependent* correlation factors. The effect related to the state dependence of the correlation is quite important, lowering the upper bound for the ground-state energy by some 2 MeV.

The physical problem of describing many interacting identical particles from a microscopic point of view can be attacked using a number of techniques. A frequent *ansatz* for the ground state (g.s.) of a many-body system is the Jastrow wavefunction. For a nuclear system the Jastrow method describes the wavefunction in terms of the product of two-body correlations between all pairs of nucleons, acting upon a suitable reference state. This approach has been very fruitful in the description of extended strongly interacting systems, such as helium liquids at zero temperature and even nuclear and neutron matter.

The practice of the Jastrow correlated method in infinite systems requires the use of massive resummation techniques, such as the hypernetted-chain (HNC) algorithms [1,2] or Monte Carlo (MC) sampling procedures [3]. After more than 20 years of practice this method has proven to be perhaps the best variational description of many-particle systems.

A different question is the treatment of finite strongly interacting systems, the main difficulty being related to the A -body interparticle correlation induced by the localization of the system. From the point of view of massive resummation of diagrams à la HNC, the most

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unpleasant fact is that any diagram becomes *elementary*, which in turn makes the HNC resummation very involved. Even though the formal equations were written many years ago [4], it is only quite recently that some results for finite nuclei with model, realistic-like, interactions have been presented [5]. On the other hand, there is no special difficulty, not present in the case of extended systems, with regard to the use of variational MC methods. In any case, the presence of state-dependent interactions and, in turn, of state-dependent correlations gives rise to a formidable computational complexity.

An alternative way to calculate expectation values for Jastrow wavefunctions consists of the consideration of *cluster expansions*, in which the mean value of an operator for an A -particle system is obtained by means of nonlinear expansions of the expectation value for n -body subsystems. As in the case of HNC and MC methods, the basic idea is taken from statistical mechanics. Cluster expansions adapted to finite systems were analysed by Clark and Westhaus [6] and used in nuclei by one of us [7]. MC studies [8], as well as the recent HNC analysis [5], have confirmed the quality of these expansions.

Previous calculations of the binding energy for several light nuclei make use of state-independent (SI) Jastrow correlations between the nucleons. Our aim is to study the effect of dealing with *state-dependent* (SD) correlation functions within a Jastrow variational context. As an initial step we will concentrate in the simple case of ^4He , as well as in simple central (but spin-isospin dependent) forces of semirealistic nature. Such interactions are usually termed as V4, the number 4 referring to the four two-body operators $\{\hat{\mathbb{1}}, \vec{\sigma}_i \cdot \vec{\sigma}_j, \vec{\tau}_i \cdot \vec{\tau}_j, (\vec{\sigma}_i \cdot \vec{\sigma}_j)(\vec{\tau}_i \cdot \vec{\tau}_j)\}$. The main difference with respect to variational MC studies is that we will carry out all calculations by means of algebraic techniques, avoiding the presence of statistical errors. This will be very important when dealing with heavier nuclei.

The trial wavefunction, formally written as $|\Psi\rangle = \hat{F}\mathcal{A}|\Phi\rangle$, is the product of a Jastrow correlation factor \hat{F} and an uncorrelated shell-model state. The latter is constructed with single-particle orbitals from the harmonic-oscillator (HO) potential, in order to be able to exactly remove the spurious centre-of-mass (CM) motion. Denoting by $\{\phi_k(x_i), k = 1, \dots, A\}$ the set of relevant normalized single-particle states (specified for the coordinates $x_i \equiv (\vec{r}_i, \vec{\sigma}_i, \vec{\tau}_i)$ of the i th nucleon), the antisymmetric reference state is nothing but the Slater determinant $\mathcal{A}|\Phi\rangle = \det(\phi_k(x_i))/\sqrt{A!}$. The Jastrow factor is the symmetrized [9,10] product of two-body correlation functions, also of V4 structure, for all pairs of nucleons. The number of factors that build up the total \hat{F} is therefore $N_C \equiv A(A-1)/2$. The correlation corresponding to a given pair (ij) is expressed as

$$\hat{f}(x_i, x_j) \equiv \hat{f}_{ij} = f^c(r_{ij}) \hat{\mathbb{1}} + f^\sigma(r_{ij}) \hat{P}_\sigma(ij) + f^\tau(r_{ij}) \hat{P}_\tau(ij) + f^{\sigma\tau}(r_{ij}) \hat{P}_\sigma(ij) \hat{P}_\tau(ij) \quad (1)$$

where the spin and isospin dependence is explicitly written in terms of spin or isospin exchange operators, and f^c, f^σ, f^τ and $f^{\sigma\tau}$ are scalar functions of the interparticle distance $r_{ij} \equiv |\vec{r}_i - \vec{r}_j|$. The SD correlated g.s. wavefunction à la Jastrow is finally written, up to a missing normalization factor, as

$$\Psi(x_1, \dots, x_A) = \mathcal{S} \left\{ \prod_{j>i=1}^A \hat{f}(x_i, x_j) \right\} \mathcal{A}\Phi(x_1, \dots, x_A) \quad (2)$$

where \mathcal{S} is the symmetrizer for the operator inside the curly brackets.

It is worth stressing that the antisymmetrization of $|\Phi\rangle$ —which is required to fulfil the fermionic nature of the nucleons— as well as the symmetrization in \hat{F} —imposed by the (in general) non-commutative character of the different pair-correlation operators— are sources of notable technical complications. From the symmetrization of $\hat{f}_{12}\hat{f}_{13}\dots\hat{f}_{A-1A}$, we see that $N_C!$ terms indeed constitute the correct, complete correlation. Then, as long as the number of particles is small the problem remains manageable but its difficulty rapidly grows with increasing A . In passing, let us mention that in most works posing this sort of treatment [10–12], the so-called independent-pair approximation¹ has widely been applied and so the question of symmetrization has been avoided.

In order to obtain the g.s. energy we should compute the mean value of the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m} \sum_{i=1}^A \nabla_i^2 + \sum_{j>i=1}^A \hat{V}(x_i, x_j) \quad (3)$$

where $\hbar^2/m = 41.47 \text{ MeV fm}^2$, and the potential \hat{V} is a two-body operator that depends on the relative spatial coordinate and the spin–isospin degrees of freedom of each pair of nucleons. The interactions employed here have V4 structure, which will be transformed to an exchange-operator basis as in the case of the correlation (1),

$$\hat{V}(x_i, x_j) = \sum_u g_u(r_{ij}) \sum_{p=1}^4 v_{u,p} \hat{O}_p(ij) \quad (4)$$

where $\hat{O}_1(ij) \equiv \hat{\mathbb{1}}$, $\hat{O}_2(ij) \equiv \hat{P}_\sigma(ij)$, $\hat{O}_3(ij) \equiv \hat{P}_\tau(ij)$ and $\hat{O}_4(ij) \equiv \hat{P}_\sigma(ij)\hat{P}_\tau(ij)$. This representation is very economical because in matrix form any exchange corresponds to a sparse matrix with a single non-null element per row and column [13]. For our calculations we will consider the quasirealistic potentials proposed by Afnan and Tang [14,15] and by Malfliet and Tjon [16], whose various components have Gauss and Yukawa spatial dependence respectively, with strengths $v_{u,p}$ and corresponding form factors $g_u^G(r) = \exp(-\mu_u r^2)$ and $g_u^Y(r) = \exp(-\mu_u r)/r$. The Coulomb interaction will not be taken into account in any case. Notice that the Hamiltonian (3) is symmetric under particle permutation and so is the operator $\hat{F}^\dagger \hat{H} \hat{F}$. This property enables us to find the total kinetic energy as A times the corresponding value for a single particle, and the total potential energy as N_C times the contribution of a single pair of nucleons.

The ${}^4\text{He}$ results presented here can be obtained exactly by a direct evaluation and further minimization of the mean value of the Hamiltonian (3) with a trial state of the form (2). Nevertheless, we have followed a cluster representation with the purpose of gaining some insight into this approach for future application to more complicated situations, namely for heavier nuclei or more realistic interactions. In that sense, the present example serves as a test for the convergence of the cluster expansion when SD correlations are taken into

¹The independent-pair approximation involves rewriting each \hat{f}_{ij} as a scalar function of r_{ij} , times an SD operator of the form $\hat{\mathbb{1}} + \hat{U}_{ij}$, and then retaining from the expansion of $\prod_{i<j}(\hat{\mathbb{1}} + \hat{U}_{ij})$ only those terms with labels that correspond to independent pairs of nucleons.

account. Besides, the approximation procedure is useful for seeking the region where the minimizing parameters of the correlation functions should be found. The methodology we followed to compute the required expectation values is the one developed in [7], that we summarize below.

Consider an n -particle subsystem ($1 \leq n \leq A$) whose Hamiltonian operator \hat{H}_n has the form (3) with the replacement $A \rightarrow n$. The n -body integrals are introduced as

$$J_n(\lambda) = \frac{1}{A(A-1)\dots(A-n+1)} \sum_{k_1, \dots, k_n=1}^A |\langle \phi_{k_1}(x_1) \dots \phi_{k_n}(x_n) | \mathcal{S} \left\{ \prod_{i' < j'}^n \hat{f}_{i'j'} \right\} e^{\lambda \hat{H}_n} \mathcal{S} \left\{ \prod_{i < j}^n \hat{f}_{ij} \right\} \sum_{P=1}^{n!} \epsilon_P |\phi_{k_1}(x_{P1}) \dots \phi_{k_n}(x_{Pn}) \rangle| \quad (5)$$

where the first sums extend over all the single-particle states relevant for the given nucleus, and the last one runs over all permutations of particle indices (ϵ_P are their associated parities). The matrix elements involve, besides spatial integrations over the whole space, summations for the spin and isospin variables of the n nucleons. If one deals with spin/isospin saturated nuclei, these summations translate into corresponding traces of products of exchange operators. Their evaluation, although quite long, can be made once at the very beginning of the calculations and the resulting values can be stored for further use (a detailed explanation on this subject can be found in [13]). In the above equation, symmetrization of an n -body correlation is required and therefore $n_C! \equiv (n(n-1)/2)!$ reorderings are obtained (both on the left and on the right), in contrast with the $N_C!$ terms arising from the complete A -particle problem. The quantity we are interested in, the minimum value acquired by $\langle \Psi | \hat{H} | \Psi \rangle / \langle \Psi | \Psi \rangle - E_{\text{CM}}$, can be derived from the A -body integral since

$$\langle \hat{H} \rangle = \left. \frac{d}{d\lambda} \ln J_A(\lambda) \right|_{\lambda=0} = \frac{J'_A(0)}{J_A(0)}. \quad (6)$$

The second term in the g.s. energy takes proper account of the CM movement and is given by the kinetic energy of a particle in the lowest HO state, i.e. $E_{\text{CM}} = 3 \hbar^2 \alpha^2 / (4m)$, α being the HO constant.

The binding energy should be obtained by scanning the space of trial correlation functions. Except for light nuclei, this is impracticable with present-day computers because of the huge number of evaluations to be performed. It proves useful to introduce a multiplicative approximation procedure by means of the *cluster integrals* \mathcal{J}_ν which are defined by the recursion

$$J_n \equiv \prod_{\nu=1}^n \mathcal{J}_\nu^{(n)} \quad (7)$$

for all $n = 1, \dots, A$. The interpretation of this chain of identities is quite straightforward: one can obtain the n -body integral as a product of different contributions arising from fewer-body interacting subsystems. This idea allows us to decompose the energy expectation value as

$$\langle \hat{H} \rangle = E^{(1)} + \sum_{\nu=2}^A \binom{A}{\nu} \delta E^{(\nu)} = A \frac{J'_1(0)}{J_1(0)} + \sum_{\nu=2}^A \binom{A}{\nu} \left. \frac{d}{d\lambda} \ln \mathcal{J}_\nu \right|_{\lambda=0}. \quad (8)$$

For a nuclear system, one may assume that a reduced number, say n , of cluster integrals would suffice in determining J_A with great accuracy, the remaining cluster integrals being close to unity so as to produce negligible contributions $\delta E^{(\nu>n)}$ to the energy (8). The A -body integral calculated up to the n th order turns out to be

$$J_A \simeq \mathcal{J}_1^A \dots \mathcal{J}_n^{(A)} \equiv J_A^{(n)} \quad (9)$$

with $\mathcal{J}_1, \dots, \mathcal{J}_n$ deduced from the recursive formulae (7). Starting with $n = 1$, one can systematically construct a series of approximations for the energy by taking the logarithmic derivatives of $J_A^{(n)}$. A detailed analysis of the characteristics and convergence of this multiplicative cluster expansion employing SI correlations has been carried out in previous works [7,8]. Up to first order the energy has purely kinetic origin and amounts to

$$E^{(1)} = \frac{\hbar^2 \alpha^2}{m} \left[3 + 5 \left(\frac{A}{4} - 1 \right) \right]. \quad (10)$$

This expression is valid for s - and p -shell nuclei, namely ${}^4\text{He}$, ${}^8\text{Be}$, ${}^{12}\text{C}$ and ${}^{16}\text{O}$, for which the spatial single-particle states are $\phi_s(\vec{r}) = (\alpha/\sqrt{\pi})^{3/2} \exp(-\alpha^2 r^2/2)$ and $\{\phi_x, \phi_y, \phi_z\}_p(\vec{r}) = \sqrt{2} \alpha \{x, y, z\} \phi_s(\vec{r})$. The first non-trivial result is obtained with one- and two-body clusters:

$$E^{(2)} = E^{(1)} + \binom{A}{2} \left[\frac{J'_2}{J_2} - 2 \frac{\mathcal{J}'_1}{\mathcal{J}_1} \right]_{\lambda=0}. \quad (11)$$

Higher orders are constructed following similar steps, i.e. calculating the successive corrections as suggested in equation (8) so that

$$E^{(n)} = E^{(n-1)} + \binom{A}{n} \delta E^{(n)}. \quad (12)$$

Let us mention that at each order one can add at once the kinetic contribution of only one of the n particles and the potential due to a given pair of them, with corresponding factors n and n_C . The approximation procedure will be performed up to a maximum of a few clusters, studying the convergence of the partial results. Note that very precise calculations are required, for two main reasons: the cancellations in $\delta E^{(n)}$ implied by the definition of \mathcal{J}_n (as the n -body integral divided by all the $\mathcal{J}_{\nu<n}$), and the fact that the statistical factors (explicitly factored out in the preceding equation) introduce an enormous scaling with n .

Let us now specify the form of the pair correlation functions. A very useful, and rather easy to handle, parametrization is an expansion in a set of Gaussians. Our *ansatz* is the SD linear combination

$$\hat{f}_{ij} = \hat{\mathbb{1}} + \sum_{m=1}^{N_\beta} e^{-\beta_m r_{ij}^2} \sum_{p=1}^4 a_{m,p} \hat{O}_p(i,j). \quad (13)$$

The correlation lengths β_m and correlation depths $a_{m,p}$, together with the HO constant α , constitute a set of (real) free parameters to be determined from energy minimization (throughout this work, distances are measured in fm and the variables β_m and α will be

given in fm^{-2} and fm^{-1} respectively). As it is clearly seen, the SI problem arises as a particular case by setting $a_{m,p \neq 1} = 0$ and freely determining the $2N_\beta + 1$ variables β_m , $a_{m,1}$ and α .

In the case of ^4He nuclei, the problem substantially simplifies due to the fact that the reference state exhibits spatial symmetry. Indeed, the uncorrelated g.s. is made up of the four particles in the same spatial single-particle state, ϕ_s . As is known, the operator $\hat{P}_\tau(ij)\hat{P}_\sigma(ij)\hat{P}_\tau(ij)$ characterizes the exchange of all coordinates of the nucleons i and j . Since $\hat{P}_\tau(ij)$ leaves the helium wavefunction unaltered, the spin and isospin exchange operators acting on $\mathcal{A}\Phi(x_1, x_2, x_3, x_4)$ give a change of sign, and consequently the action of \hat{P}_σ is equivalent to minus that of \hat{P}_τ . The same holds in second and third order of the cluster expansion for ^4He . Then, for this nucleus we are able to rewrite the correlation factors with a simpler state dependence, the *ansatz* (13) becoming

$$\hat{f}_{ij} = \hat{1} + \sum_{m=1}^{N_\beta} e^{-\beta_m r_{ij}^2} [a_{m,c} \hat{1} + a_{m,\sigma} \hat{P}_\sigma(ij)] \quad (14)$$

with central scalar and spin-exchange constituents only. The state-independent study is performed, as usual, by setting $a_{m,\sigma} = 0$ for all m .

In tables I and II we present the results corresponding to the g.s. energy of the ^4He nucleus, obtained using different trial wavefunctions and nucleon–nucleon interactions. Table I corresponds to the Afnan–Tang S3 potential [14] and its modified version MS3 [15], while in table II the Malfliet–Tjon interactions MT I/III and MT V [16] are considered. The four-particle system has been characterized by a Jastrow prescription with state-dependent correlations containing one and two Gaussian components. For the sake of comparison, we also show in the tables the concomitant state-independent energies (the SI values have earlier been computed in [17] assuming $\hbar^2/m = 41.50 \text{ MeV fm}^2$). Together with the minima obtained in each case, we exhibit the optimum values for the HO constant α , correlation lengths β_m and correlation depths $a_{m,c}$ and $a_{m,\sigma}$, for $m \leq N_\beta$ with $N_\beta = 1$ and 2.

The S3 potential is parametrized in terms of five ranges μ_u and has only singlet–even and triplet–even channels; the MS3 interaction incorporates the odd ones. Although for helium both potentials yield the same results employing SI pair correlation factors, the introduction of a dependence upon the spin of the nucleons distinguishes between those interactions. The MS3 shift with respect to the SI binding energy turns out to be somewhat smaller in magnitude than the S3 one: 3.7% (9.1%) against 3.9% (10.0%) respectively, for one (two) correlation lengths. This difference is related to the saturation properties of the modified Afnan–Tang interaction.

The potentials proposed by Malfliet and Tjon are a superposition of an attractive and a repulsive Yukawa component. In the MT I/III case, the spin-singlet and spin-triplet even channels are split; for the MT V case it is assumed that these two forces can be replaced by an average effective potential which is identical in both channels. The last situation allows one to treat the four nucleons as identical spinless bosons, meaning that the SI and SD approaches for the MT V potential give the same result, which is also consistent with the state-independent treatment for the MT I/III force. We find that with this interaction the state-dependent binding energy diminishes by almost 1% (3.7%) of the SI value for $N_\beta = 1$ ($N_\beta = 2$).

The results presented here can be compared with other existing calculations, among which we may mention the energies given using MC techniques and the spin–isospin-dependent translationally invariant coupled cluster (TICI2) treatment [13]. In the case of the MT V potential, for instance, our ($N_\beta = 2$)-result is very close to the Green function MC value of (-31.3 ± 0.2) MeV [18] and the diffusion MC energy, (-31.32 ± 0.02) MeV [17]. After performing a coupled cluster calculation for the alpha particle, Zabolitzky [19] arrived at the conclusion that the g.s. eigenvalue of the MT I/III Hamiltonian should be (-33.4 ± 0.1) MeV. The TICI2 method with SD linear correlations of the V4 type yields the following results [13] for the quoted potentials: -28.19 MeV (S3), -27.99 MeV (MS3), -30.81 MeV (MT I/III) and -29.45 MeV (MT V). These values have not been optimized with respect to the HO parameter and hence they may be slightly underestimated in magnitude. It can be seen that the results given here are comparable with the binding energies of the TICI2 method; moreover, our results with two betas are lower than the latter by more than 1 MeV.

In order to look at the convergence of the above mentioned multiplicative cluster expansion, we show the partial results corresponding to the minimum energies found with one and two β parameters. Table III contains for $N_\beta = 1$ the first-order energy $E^{(1)}$ as well as the concomitant corrections up to the second, third and fourth orders, which should be multiplied by the statistical factors 6, 4 and 1 respectively. One can see that in this situation the SI fourth-order corrections are much smaller than the respective third-order terms, and using SD correlation functions $|\delta E^{(4)}|$ remains lower than $|\delta E^{(3)}|$; finally, the third- and fourth-order corrections have opposite signs. The influence of the introduction of a second SD correlation component is shown in table IV, giving evidence that in this case four-body SD contributions gain in importance and thus are not negligible. Moreover, for the MT potentials the third- and fourth-order corrections both contribute to lower the second-order energy. We stress that, at this step, our purpose is to compare the minimum total energy with the third-order approximation obtained assuming the optimum parametrization of tables I and II, which in principle should not be equal to the minimum $E^{(3)}$.

In conclusion, let us remark on the good agreement of our results with the available MC ones, when we take into account just two correlation components. We have shown the importance of introducing a dependence with the spin and isospin of the nucleons in the pair correlation functions, the shift in the energies with respect to the state-independent values being of around 1–10%, depending on the two-body interaction considered. As a side benefit, in this simple case of helium nuclei we were able to test the convergence of the multiplicative cluster expansion, a crucial treatment to be taken into account for the study of heavier systems because the ‘size’ of the problem is considerably reduced with respect to the full energy computation. We note that, at least in the case of ^4He , the fourth-order contribution to the binding energy is non-negligible for the (SD, $N_\beta = 2$) approach.

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TABLES

| Potential | Correlation | Energy | α | β_m | $a_{m,c}$ | $a_{m,\sigma}$ |
|-----------|-------------------|----------|----------|------------------------|-------------------|-------------------|
| S3, MS3 | SI, $N_\beta = 1$ | -24.4042 | 0.8293 | 2.0502 | -0.7191 | — |
| S3 | SD, $N_\beta = 1$ | -25.3598 | 0.8380 | 1.9433 | -0.7012 | 0.1128 |
| MS3 | SD, $N_\beta = 1$ | -25.3119 | 0.8373 | 1.9486 | -0.7023 | 0.1073 |
| S3, MS3 | SI, $N_\beta = 2$ | -27.2136 | 0.5795 | 1) 1.6206 2) 0.2402 | -1.5596 1.0872 | — — |
| S3 | SD, $N_\beta = 2$ | -29.9378 | 0.6617 | 1) 1.4646 2) 0.3892 | -1.4704 0.9511 | -0.2805 0.4877 |
| MS3 | SD, $N_\beta = 2$ | -29.7034 | 0.6570 | 1) 1.4703 2) 0.3765 | -1.4617 0.9413 | -0.2454 0.4409 |

TABLE I. For the Afnan–Tang potentials, g.s. energy of a ^4He nucleus and optimum correlation parameters for different situations (energies are given in MeV, α in fm^{-1} and β_m in fm^{-2}).

| Potential | Correlation | Energy | α | β_m | $a_{m,c}$ | $a_{m,\sigma}$ |
|----------------|-------------------|----------|----------|------------------------|-------------------|-------------------|
| MT I/III, MT V | SI, $N_\beta = 1$ | -29.0604 | 0.8174 | 3.8314 | -0.7934 | — |
| MT I/III | SD, $N_\beta = 1$ | -29.3460 | 0.8201 | 3.7559 | -0.7853 | -0.0642 |
| MT I/III, MT V | SI, $N_\beta = 2$ | -30.8752 | 0.5089 | 1) 3.4460 2) 0.1455 | -1.9090 1.4125 | — — |
| MT I/III | SD, $N_\beta = 2$ | -32.0107 | 0.6077 | 1) 3.3441 2) 0.2018 | -1.4139 0.8203 | 0.2230 -0.3998 |

TABLE II. Same considerations of table I, for the potentials proposed by Malfliet and Tjon. For the MT V interaction, being of Wigner type, the SD approach gives the same binding energy as the SI one, i.e. the optimum $a_{m,\sigma}$ are zero.

| Potential | Correlation | $E^{(1)}$ | $\delta E^{(2)}$ | $\delta E^{(3)}$ | $\delta E^{(4)}$ |
|----------------|-------------|-----------|------------------|------------------|------------------|
| S3, MS3 | SI | 85.5600 | -15.5220 | 1.1913 | -0.2076 |
| S3 | SD | 87.3595 | -16.0471 | 1.4832 | -0.5300 |
| MS3 | SD | 87.2105 | -16.0198 | 1.4785 | -0.5151 |
| MT I/III, MT V | SI | 83.1312 | -15.6007 | 0.5628 | -0.0559 |
| MT I/III | SD | 83.6763 | -15.7429 | 0.6180 | -0.1178 |

TABLE III. Contributions (given in MeV), up to all cluster orders, to the minimum g.s. energy for both Afnan–Tang and Malfliet–Tjon interactions and the optimal one-beta parametrizations. The CM corrections have not been included.

| Potential | Correlation | $E^{(1)}$ | $\delta E^{(2)}$ | $\delta E^{(3)}$ | $\delta E^{(4)}$ |
|----------------|-------------|-----------|------------------|------------------|------------------|
| S3, MS3 | SI | 41.7835 | -8.1422 | -2.4407 | 0.0645 |
| S3 | SD | 54.4792 | -11.7120 | 0.7360 | -3.4694 |
| MS3 | SD | 53.7015 | -11.5075 | 0.5723 | -3.2238 |
| MT I/III, MT V | SI | 32.2192 | -6.7370 | -3.6119 | -0.1697 |
| MT I/III | SD | 45.9464 | -10.3470 | -0.0580 | -4.1564 |

TABLE IV. Same considerations of table III, for the optimal two-beta parametrizations.